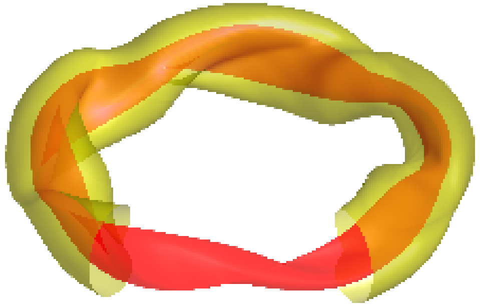
An adjoint method for gradient-based optimization of stellarator coil shapes



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PPPL Theory Seminar
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Outline

1. Introduction
2. Current potential approach for coil optimization
   a) NESCOIL
   b) REGCOIL
3. Nonlinear optimization of the winding surface
   a) Objective function
   b) Optimization constraints
4. Adjoint method for gradient computation
   a) Examples from CFD and electron gun optimization
   b) Linear adjoint method
5. Applications
   a) Optimization of W7-X and HSX winding surfaces
6. Local sensitivity analysis

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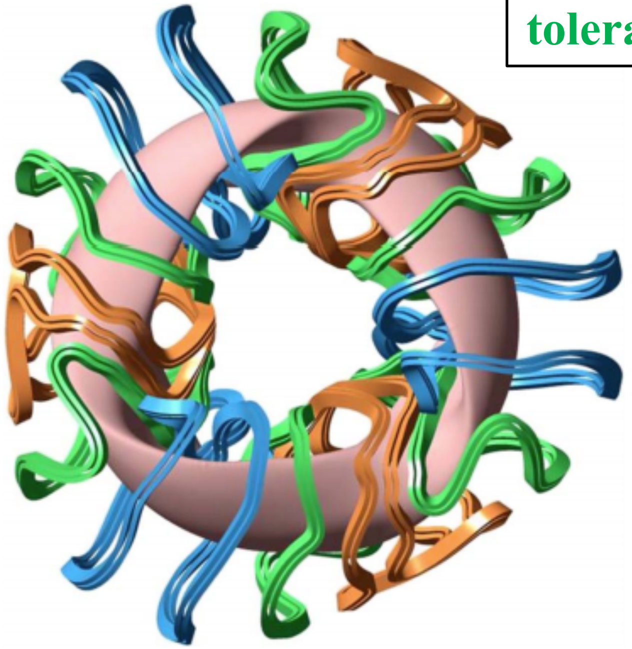
Designing & constructing 3-D coils is challenging

The construction of the National Compact Stellarator Experiment (NCSX) was never completed, party due to increasing costs and **small tolerances** in producing the magnetic field



Modular coil set for NCSX [3]

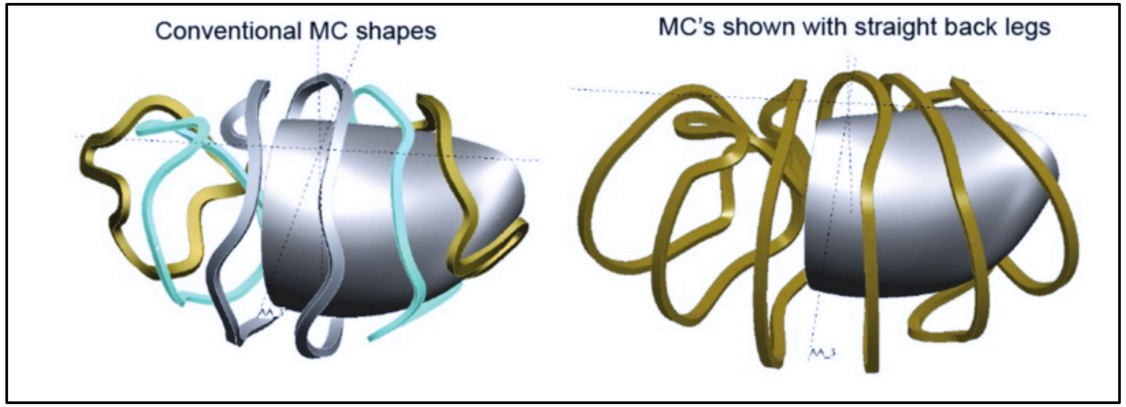
How can we more successfully design stellarator coils?

- Stellarators are fully 3-D, so design space is extremely large
- Large **non-linear optimizations** are now used in the design process
- First step in optimization: identify plasma shape and configuration with good physics properties (MHD stability, neoclassical & turbulent transport)
- Coils chosen to minimize error in producing magnetic surfaces desired
- Many desirable engineering considerations
  - Sufficient space between coils and plasma to allow for neutron shielding and blanket
  - Sufficient coil-coil spacing for maintenance, diagnostics, and neutral beams
  - Small curvature to allow for finite thickness of conducting material
  - Small bending ($\boldsymbol{J} \times \boldsymbol{B}$) forces on coils (less support required)
- **Coil design is closely tied to cost and size of stellarator**

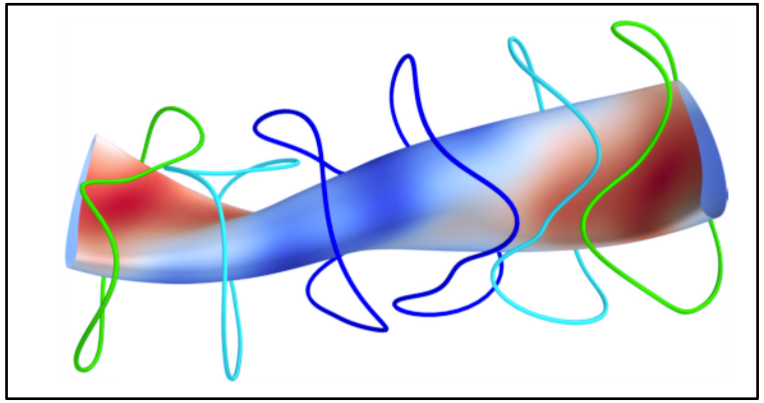
Coil optimization tools

- Nonlinear optimization codes – not guaranteed to find global minimum, requires tuning of weighting parameters
  - COILOPT++
    - Coils represented by splines on winding surface
  - FOCUS
    - Coils represented by 3D space curves (no winding surface)
- Current potential methods – robust and fast, but do not include finite coil effects
  - NESCOIL
  - REGCOIL
- Coil optimization is difficult - **important to have multiple tools**

COILOPT++ allows 'straightening' of modular coils [14]



W7-X modular coils optimized with FOCUS [15]



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Finding coil shapes on a winding surface

Given a fixed winding surface and plasma surface, how should I design my coils?

W7-X plasma surface (red) and coil-winding surface (green) [5]

- One of the earliest methods (NESCOIL [4]) used for stellarator coil design assumed all coils to lie on a winding surface (toroidal surface enclosing plasma)
- Plasma surface is fixed based on physics optimization
- Divergentless current density on a surface can be computed from current potential, Φ
- Contours of Φ give coil shapes (streamlines of $\boldsymbol{K}$)

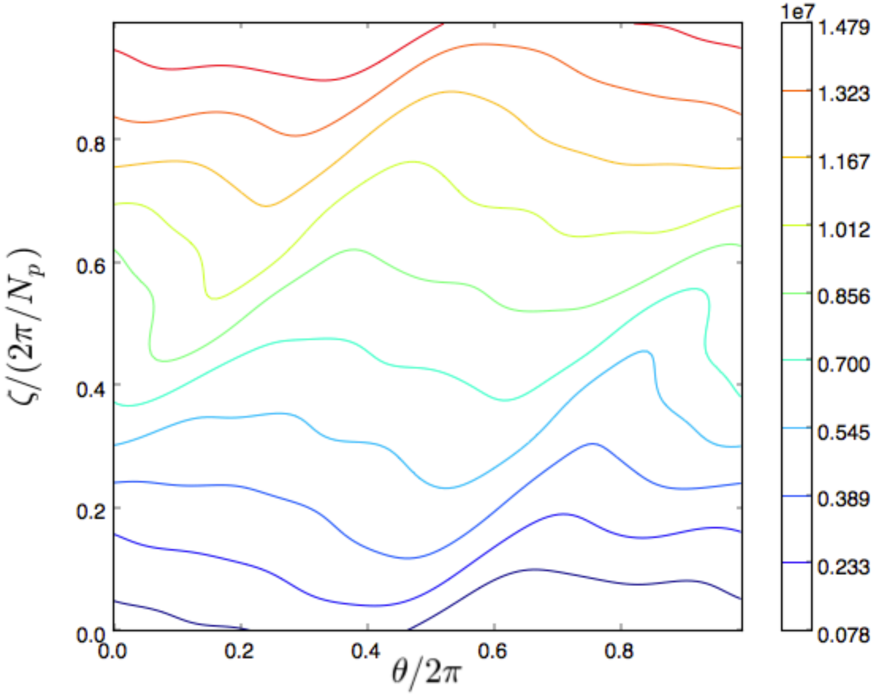
$$\boldsymbol{K} = \underset{\substack{\uparrow \\ \text{Unit normal on coil surface}}}{\boldsymbol{n}} \times \nabla \Phi$$

Current potential is composed of secular terms, determined by net poloidal and toroidal surface currents, and single-valued (periodic) piece which we optimize

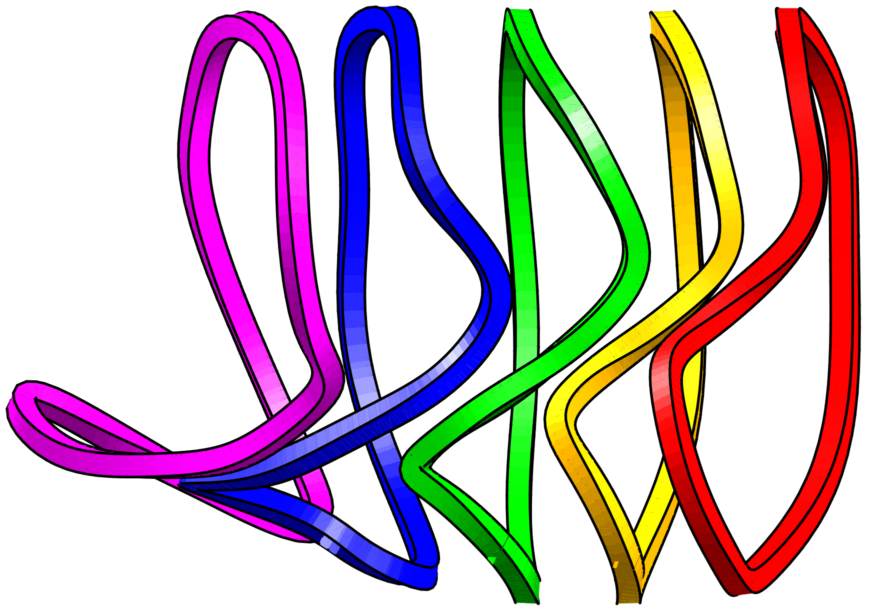
$$\Phi = \underbrace{\Phi_{\text{sv}}}_{\text{single-valued}} + \overbrace{\frac{G\zeta}{2\pi} + \frac{I\theta}{2\pi}}^{\text{Determined by net currents linking plasma}}$$

Example – Current potential for W7-X modular coil set

Total current potential

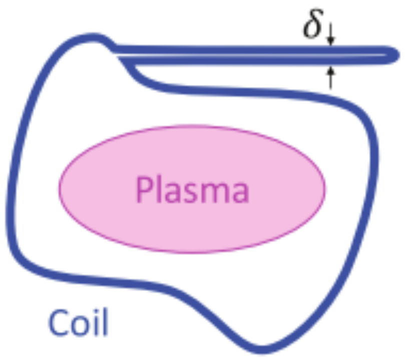


Corresponding coil set (1/2 period)



REGCOIL [5] approach

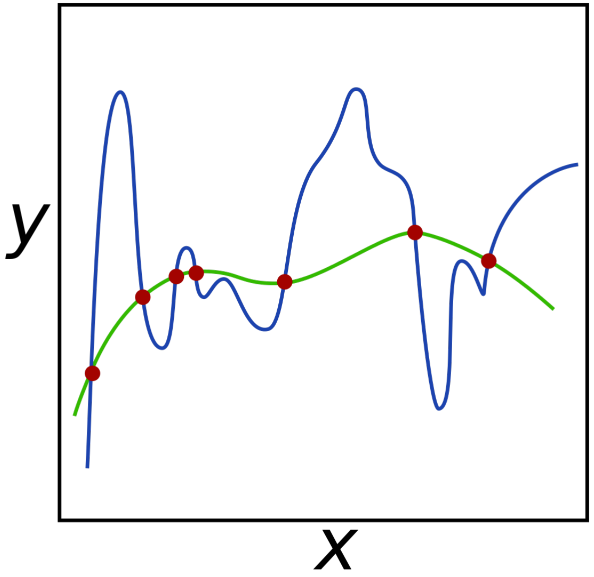
- REGCOIL [5] is a current potential method which applies **Tikhonov regularization**
- Solves ill-posed problem: very different current distributions can give nearly identical magnetic surfaces
- Improves condition number of linear least-squares problem
- Simultaneously **improves engineering properties** of coils



Tikhonov regularization

$$\min_{\boldsymbol{x}} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\| + \|\boldsymbol{\Gamma}\boldsymbol{x}\|$$

Analogous to polynomial fitting – overfitting amplifies noise



REGCOIL regularization

$$\min_{\Phi} \underbrace{\chi_B^2}_{} + \lambda \underbrace{\chi_K^2}_{}$$

Fidelity in reproducing plasma surface

$$\chi_B^2 = \int_{\text{plasma}} d^2A \, B_n^2$$

If plasma surface were exactly reproduced, $\chi_B^2 = 0$

Increased coil-coil spacing

$$\chi_K^2 = \int_{\text{coil}} d^2A \, K^2$$

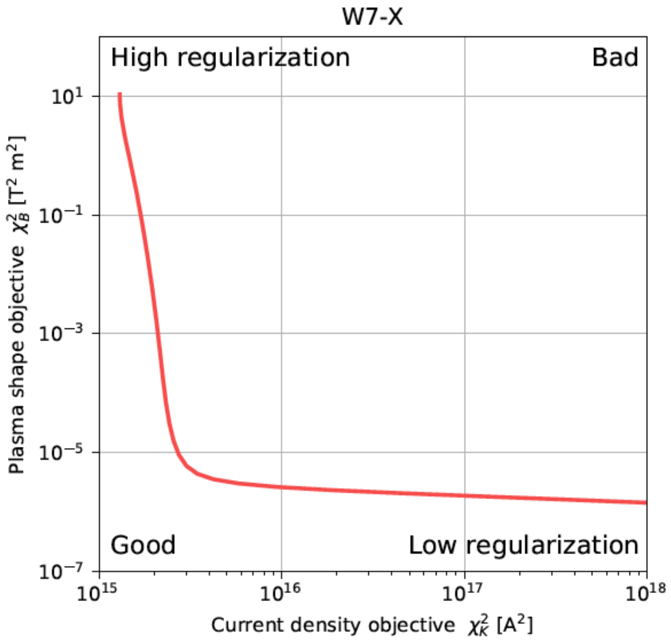
REGCOIL [5] approach

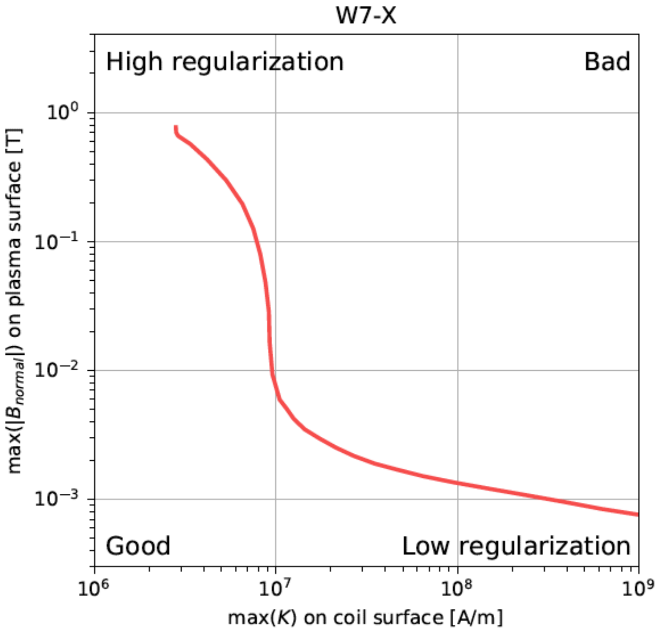
$$\Phi_{sv} = \sum_{m,n} \Phi_{mn} \sin(m\theta - n\zeta)$$

- Φ_{sv} expanded in sine series (assuming stellarator symmetry)
- For NESCOIL ($\lambda = 0$), only regularization provided by truncation of Fourier series

Our task: $\min_{\Phi} \chi^2 = \chi_B^2 + \lambda \chi_K^2$ → **Linear least-squares problem**

$$\boldsymbol{A\Phi = b}$$



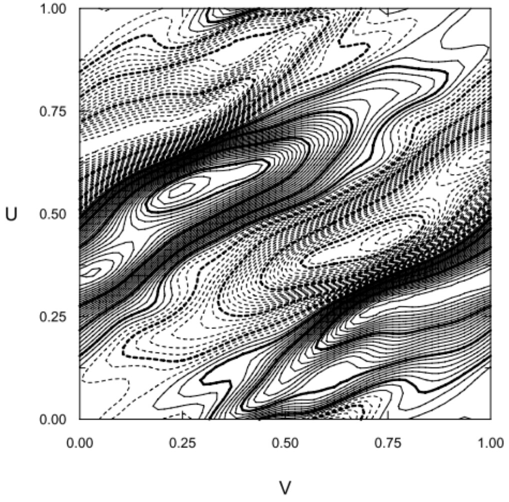


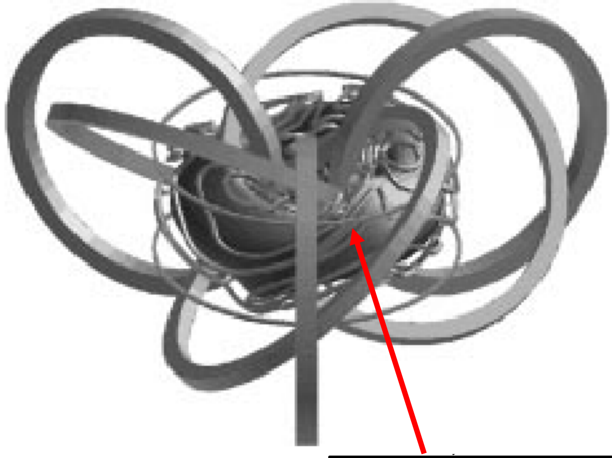
- Tradeoff between low field error and low current density
- Regularization (λ) chosen to meet some prescribed tolerance
  - e.g., K_{max} (coil-coil spacing)
  - Obtained from numerical root-finding algorithm

The current potential method has been widely applied

- **Robust**: guaranteed to find a minimum
- **Fast**: requires inverting a matrix of size $\lesssim 144 \times 144$
- For these reasons, often **used in initial stages of coil optimization process**

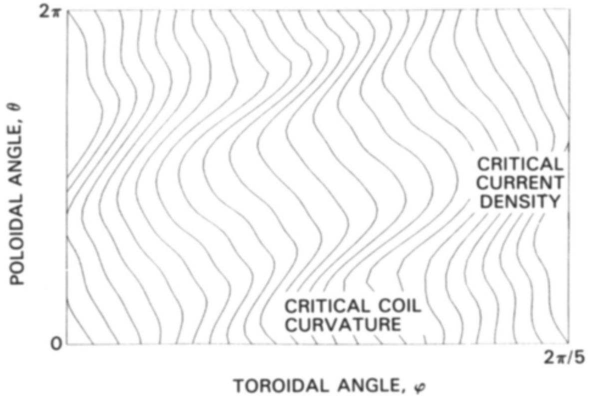
Contours of the current potential and coil set obtained with NESCOIL in initial NCSX design [6]

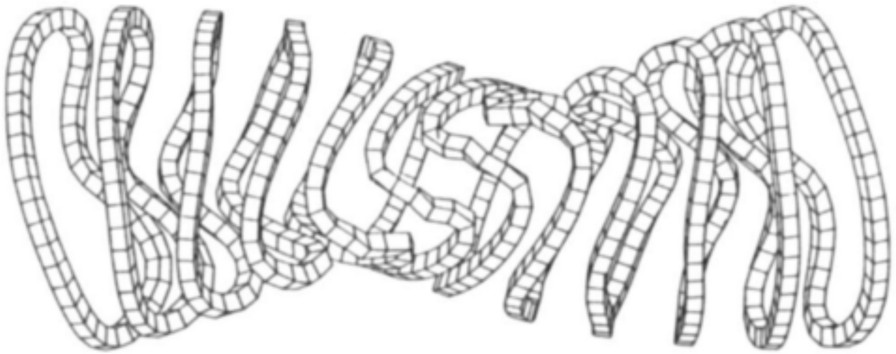




Winding surface

W7-X coils obtained from NESCOIL with modified winding surface [12]





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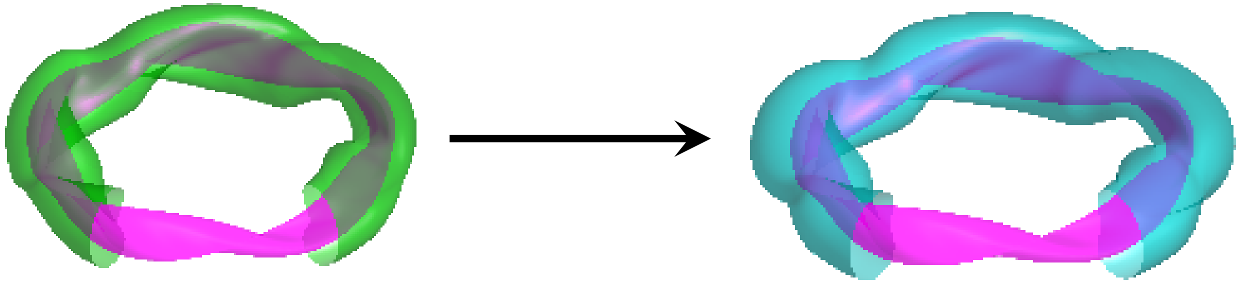
Optimization of the winding surface

- Compute the current distribution on fixed winding surface using REGCOIL
- We'd like to find the optimum **coil shapes in 3D space** rather than on a fixed surface – this amounts to optimizing the winding surface
- Plasma surface is fixed
- Properties we'd like in a winding surface:
  - Fidelity in **producing desired plasma surface**
  - **Maximize space** between coil surface and plasma surface
  - Allows for **simple coils**



Optimization parameters: $\Omega = \{r^c_{mn}, z^s_{mn}\}$

$$x = \sum_{m,n} r^c_{mn} \cos(m\theta - n\zeta)\cos\zeta$$

$$y = \sum_{m,n} r^c_{mn} \cos(m\theta - n\zeta)\sin\zeta$$

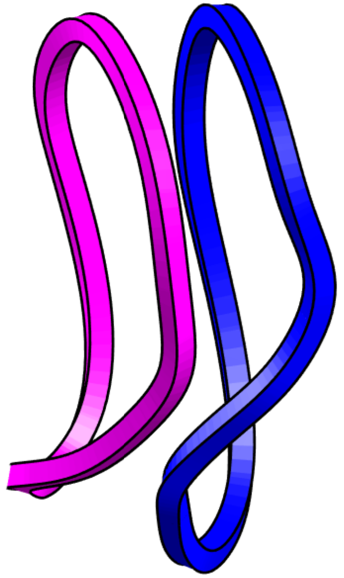
$$z = \sum_{m,n} z^s_{mn} \sin(m\theta - n\zeta)$$

Cartesian components of winding surface

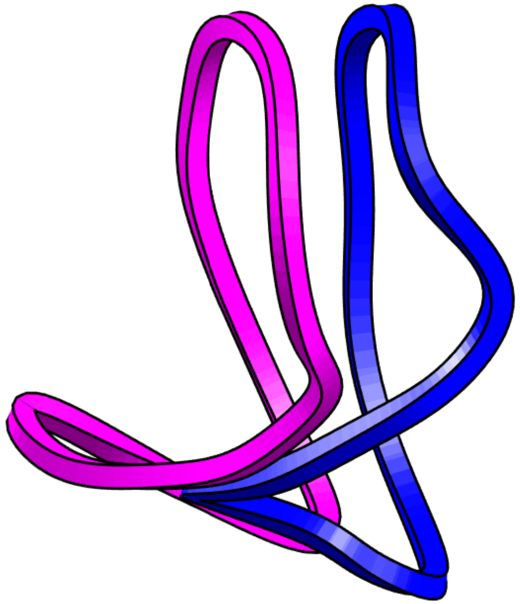
Current density is a proxy for coil complexity

Coils computed on same winding surface (only λ varying)

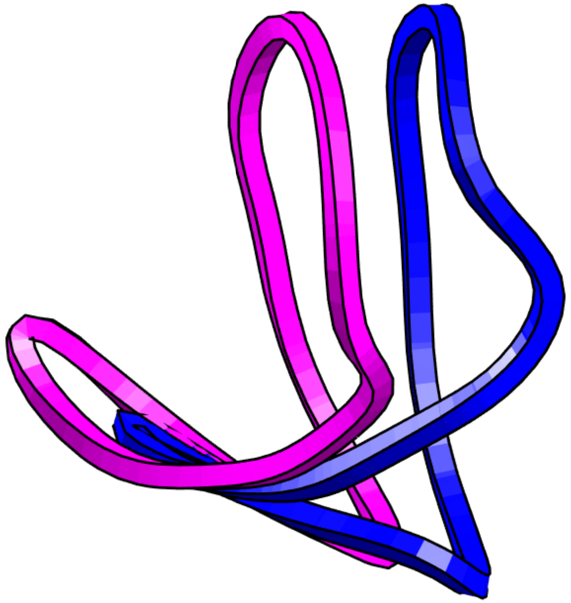
$\|\boldsymbol{K}\|_2 = 2.2$ MA/m



$\|\boldsymbol{K}\|_2 = 2.7$ MA/m



$\|\boldsymbol{K}\|_2 = 3.2$ MA/m



Increasing coil complexity →

- Increased maximum current density
- Increased coil length
- Increased toroidal extent
- Increased curvature
- Decreased coil-coil spacing

Objectifying our optimization

Our task: $\min_{\Omega} f$

$$f(\Omega, \mathbf{\Phi}(\Omega)) = \underbrace{\chi^2_B(\Omega, \mathbf{\Phi}(\Omega))}_{\text{Fidelity in reproducing plasma surface}} - \underbrace{\alpha_V V_{\text{coil}}^{1/3}(\Omega)}_{\text{Increase coil-plasma distance}} + \underbrace{\alpha_S S_p(\Omega)}_{\text{Represent surface with a condensed Fourier series}} + \alpha_K \overbrace{\|\boldsymbol{K}\|_2}^{\text{Decrease coil complexity}} (\Omega, \mathbf{\Phi}(\Omega))$$

Decrease coil complexity

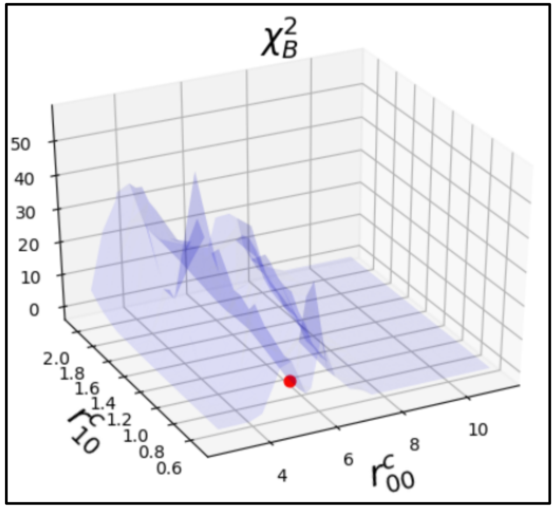
Fidelity in reproducing plasma surface

Increase coil-plasma distance

Represent surface with a condensed Fourier series

$$S_p = \sum_{m,n} m^p \left(\left(r^c_{mn}\right)^2 + \left(z^s_{mn}\right)^2 \right)$$

- We want to use a **gradient-based optimization** method to minimize f
- V_{coil} and S_p are only functions of geometry, so can be explicitly differentiated with respect to Ω
- Gradient of χ^2_B could be computed by finite differencing
  - This could be prohibitively expensive – requires $N_\Omega + 1$ (≈ 100) calls to REGCOIL
- Alternatively, use the ***adjoint method*** - only requires 2 calls to REGCOIL



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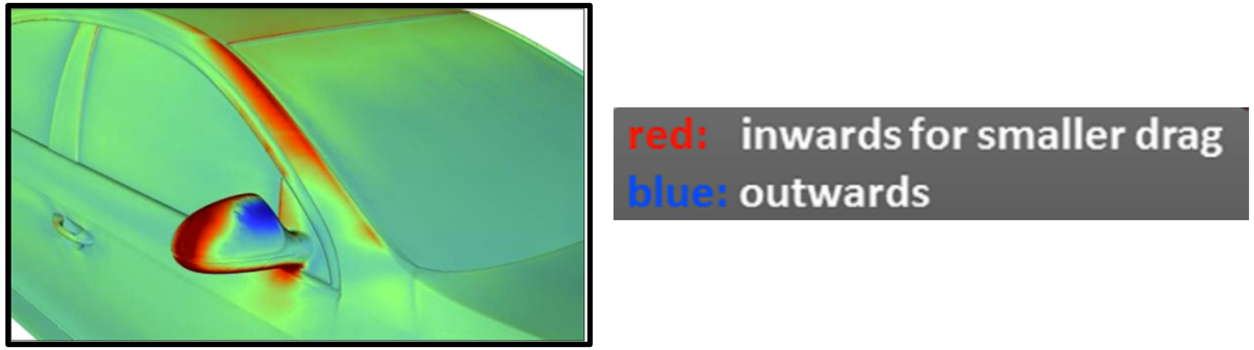
What is an adjoint method?

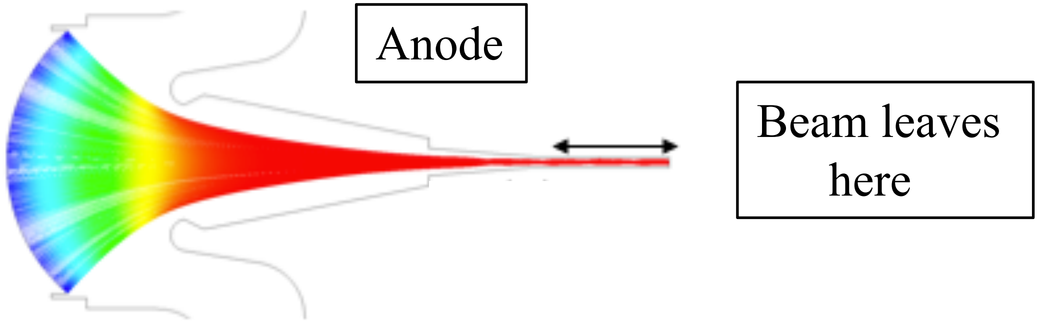
- Allow for **efficient computation of gradients** of output quantities of a linear or non-linear solve **with respect to input parameters**
- Solve an adjoint (“backward in time”) equation in addition to original (“forward”) equation
- Developed in 1970s for analysis of drag and flow dynamics
- Widely used in computational fluid dynamics and aerodynamic engineering
- Applications
    - Gradient-based optimization
    - Uncertainty quantification in scientific computing
    - Surface sensitivity maps

CFD Shape optimization



How does the total drag depend on the shape of the mirror on the VW Passat? [7]

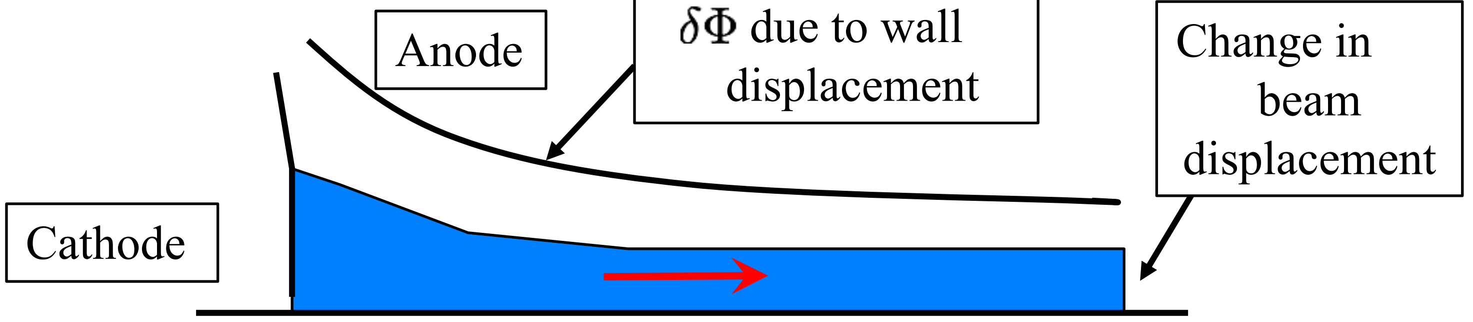
Electron gun sensitivity



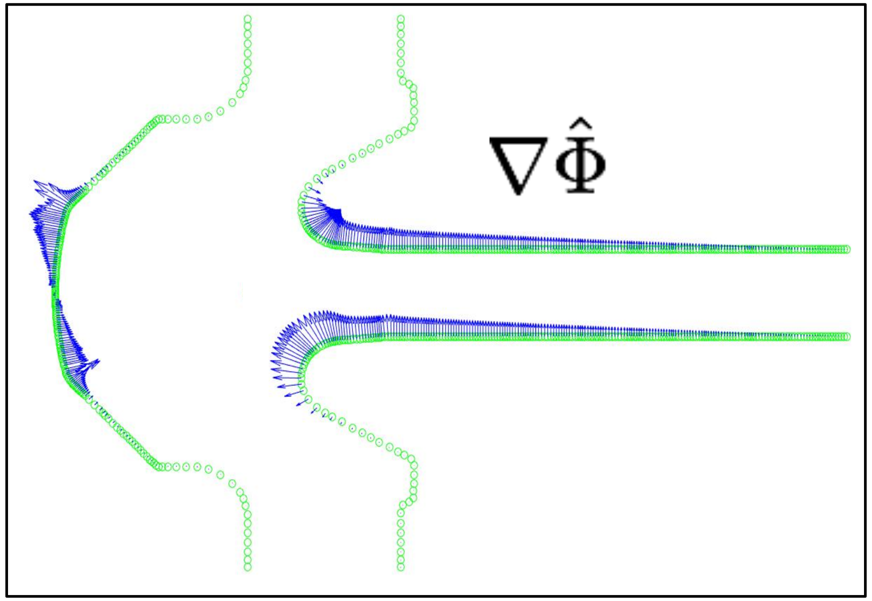
What is the sensitivity of the displacement of the beam to the properties of the anode? [8]

Example: Adjoint method for electron gun design [11]

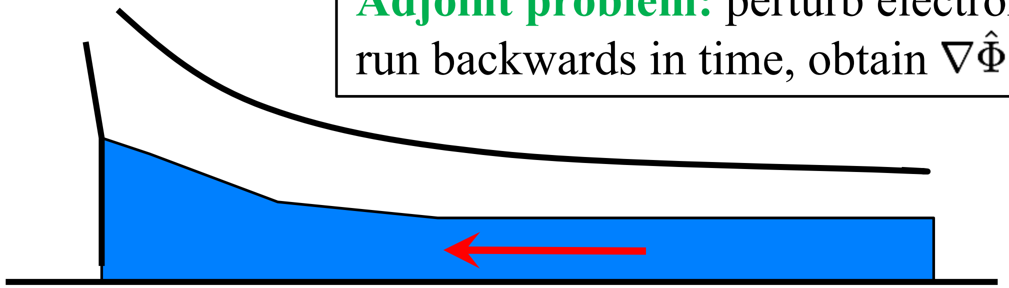
Question: How do small changes in position or potential of anode affect the properties of the beam leaving the gun?



Vector plot of the sensitivity function of the beam displacement to local changes in electric potential



Adjoint problem: perturb electron positions and run backwards in time, obtain $\nabla\hat{\Phi}$



$$\delta x \propto \int_{\text{anode}} d^2A \left(\boldsymbol{n}\cdot\nabla\hat{\Phi}\right)\delta\Phi$$

Displacement of beam

'Sensitivity function' (from backward problem)

Local change in electric potential

Adjoint method for a linear system

We'd like to compute the gradient of some function of input and output parameters

$$\left.\frac{\partial f(\Omega_i, \boldsymbol{x}(\Omega_i))}{\partial \Omega_i}\right|_{\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b}} = \left.\frac{\partial f}{\partial \Omega_i}\right|_{\boldsymbol{x}} + \left(\frac{\partial f}{\partial \boldsymbol{x}}\right) \cdot \left.\frac{\partial \boldsymbol{x}}{\partial \Omega_i}\right|_{\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b}}$$

State variable, $\boldsymbol{x}$, satisfies linear "forward" equation and depends on **many input parameters**, $\Omega = \{\Omega_i\}$

$$\boldsymbol{A}(\Omega_i)\boldsymbol{x} = \boldsymbol{b}(\Omega_i)$$

Differentiate with respect to Ω_i

$$\frac{\partial \boldsymbol{A}}{\partial \Omega_i}\boldsymbol{x} + \boldsymbol{A}\frac{\partial \boldsymbol{x}}{\partial \Omega_i} = \frac{\partial \boldsymbol{b}}{\partial \Omega_i} \rightarrow \left.\frac{\partial \boldsymbol{x}}{\partial \Omega_i}\right|_{\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b}} = \boldsymbol{A}^{-1}\underbrace{\left(\frac{\partial \boldsymbol{b}}{\partial \Omega_i} - \frac{\partial \boldsymbol{A}}{\partial \Omega_i}\boldsymbol{x}\right)}_{c(\boldsymbol{x},\Omega_i)}$$

Insert the expression for $\left.\frac{\partial \boldsymbol{x}}{\partial \Omega_i}\right|_{\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b}}$

$$\left.\frac{\partial f(\Omega_i, \boldsymbol{x}(\Omega_i))}{\partial \Omega_i}\right|_{\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b}} = \left.\frac{\partial f}{\partial \Omega_i}\right|_{\boldsymbol{x}} + \left(\frac{\partial f}{\partial \boldsymbol{x}}\right) \cdot \left[\boldsymbol{A}^{-1}\boldsymbol{c}(\boldsymbol{x}, \Omega_i)\right]$$

This requires inverting A for each Ω_i we'd like to differentiate with respect to!

Adjoint method for a linear system

We'd like to compute the derivative for many Ω_i

$$\left.\frac{\partial f(\Omega_i, \boldsymbol{x}(\Omega_i))}{\partial \Omega_i}\right|_{\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b}} = \left.\frac{\partial f}{\partial \Omega_i}\right|_{\boldsymbol{x}} + \left(\frac{\partial f}{\partial \boldsymbol{x}}\right) \cdot \left[\underbrace{\boldsymbol{A}^{-1}\boldsymbol{c}(\boldsymbol{x}, \Omega_i)}\right]$$

Invert N_Ω times!

We'll exploit the adjoint property for this inner product $(\boldsymbol{A}^T\boldsymbol{b}, \boldsymbol{c}) = (\boldsymbol{b}, \boldsymbol{A}\boldsymbol{c})$

$$\left.\frac{\partial f(\Omega_i, \boldsymbol{x}(\Omega_i))}{\partial \Omega_i}\right|_{\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b}} = \left.\frac{\partial f}{\partial \Omega_i}\right|_{\boldsymbol{x}} + \left[\left(\boldsymbol{A}^T\right)^{-1}\left(\frac{\partial f}{\partial \boldsymbol{x}}\right)\right] \cdot \boldsymbol{c}(\boldsymbol{x}, \Omega_i)$$

We can instead invert the adjoint operator once

$$\boldsymbol{A}^T\boldsymbol{q} = \frac{\partial f}{\partial \boldsymbol{x}}$$

We take an an inner product for each Ω_i we'd like to differentiate with respect to

$$\left.\frac{\partial f(\Omega_i, \boldsymbol{x}(\Omega_i))}{\partial \Omega_i}\right|_{\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b}} = \left.\frac{\partial f}{\partial \Omega_i}\right|_{\boldsymbol{x}} + \boldsymbol{q} \cdot \boldsymbol{c}(\boldsymbol{x}, \Omega_i)$$

- Assuming that inverting $\boldsymbol{A}$ is the computational bottleneck, the adjoint method **scales independently of the number of input parameters** you are differentiating with respect to (requires 2 linear solves)
- Can be generalized to non-linear systems and general inner product spaces

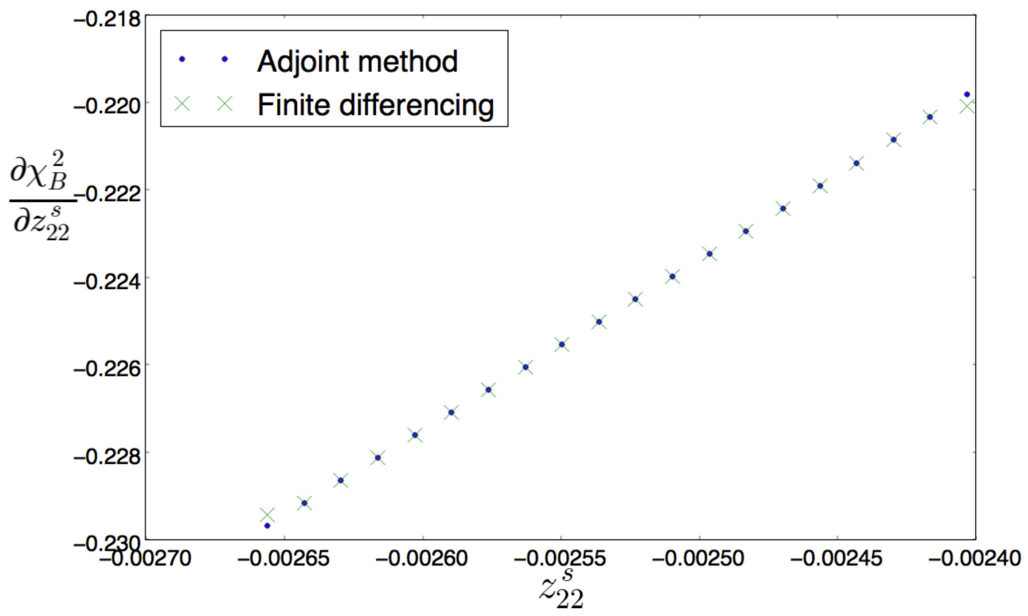
Putting adjoint methods to the test in REGCOIL

We use the linear adjoint method to obtain

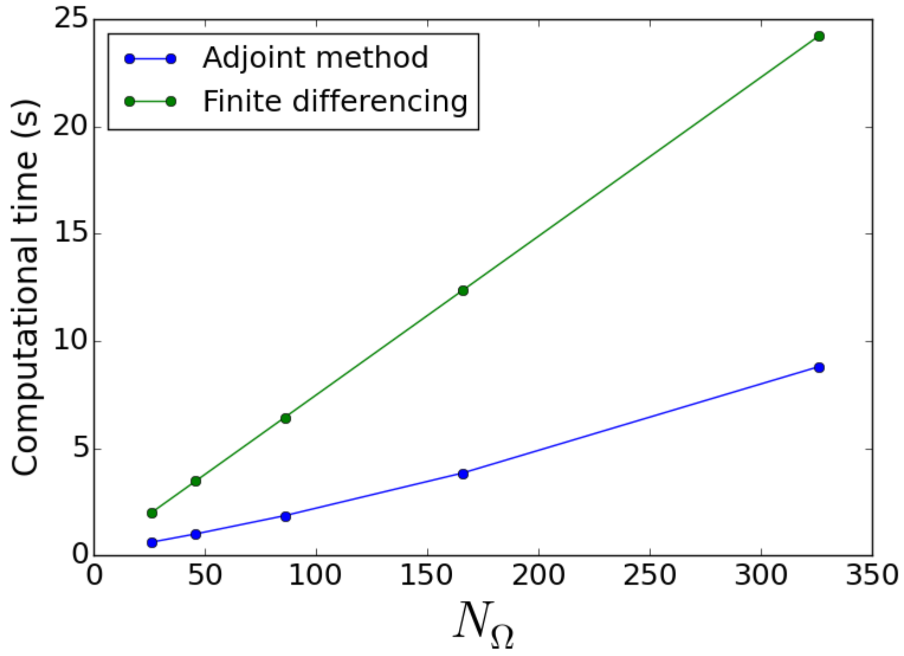
$$\left\{ \frac{\partial \chi_B^2}{\partial \Omega}, \frac{\partial \|\boldsymbol{K}\|_2}{\partial \Omega} \right\}$$

Forward equation	Adjoint equation
$\boldsymbol{A}\boldsymbol{\Phi} = \boldsymbol{b}$	$\boldsymbol{A}^T \boldsymbol{q} = \frac{\partial \chi_B^2}{\partial \boldsymbol{\Phi}}$

Benchmark with finite difference derivatives



Computational time scaling

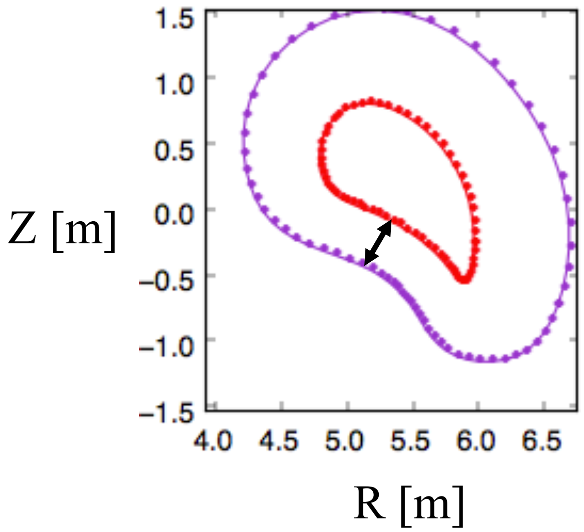


Optimization constraints

Inequality constraint on minimum coil-plasma distance

$$d_{\text{min}} = \min_{\theta,\zeta} \left(d_{\text{coil-plasma}} \right)$$

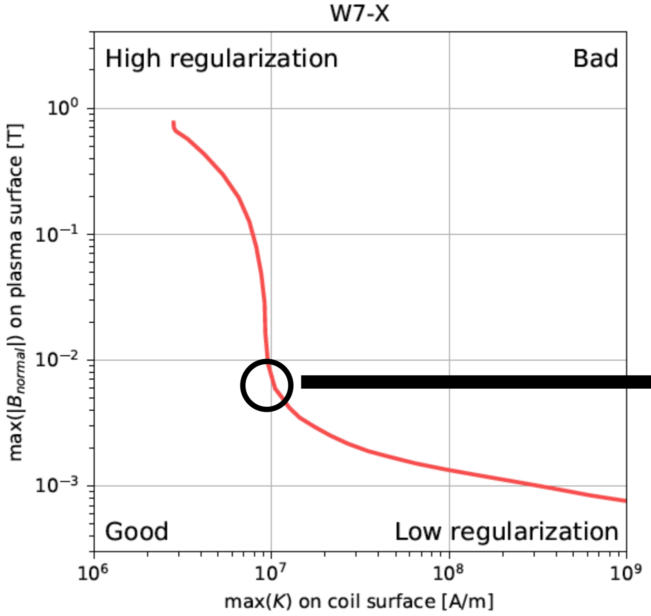
$$d_{\text{min}} \geq d_{\text{min}}^{\text{target}}$$

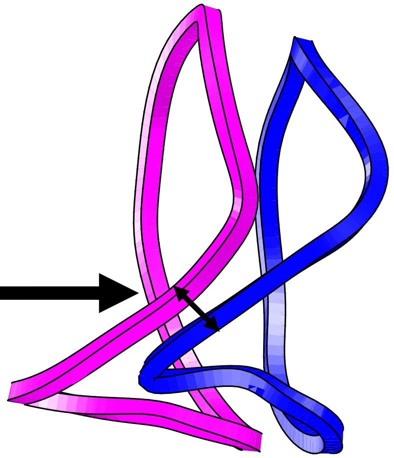


Regularization, λ, chosen to fix maximum current density

$$\chi^2 = \chi_B^2 + \lambda \chi_K^2$$

Corresponds to fixed coil-coil spacing





Gradient-based optimization of objective function

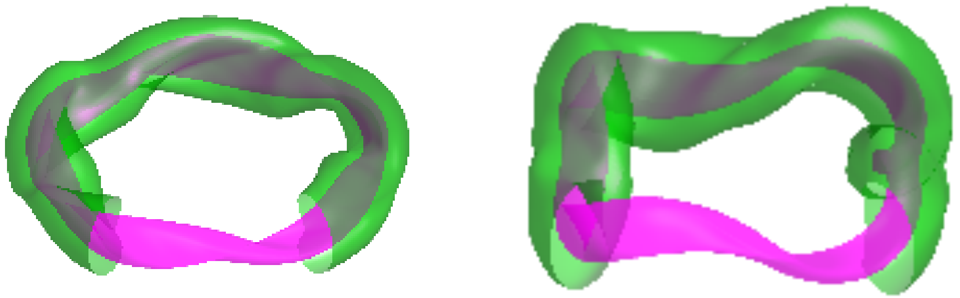
$$f(\Omega, \mathbf{\Phi}(\Omega)) = \chi^2_B + \alpha_K \|\boldsymbol{K}\|_2 - \alpha_V V_{\text{coil}}^{1/3} + \alpha_S S_p$$

Gradients can be computed with the linear adjoint method

Analytically differentiate

- We use the sequential linear-squares quadratic programming (SLSQP) for constrained optimization
  - Implementation in NLOPT package
- For demonstration, begin with actual HSX and W7-X winding surfaces

Can we design 'better' winding surfaces?



Remaining challenge:
How do we choose α_V, α_S, and α_K?

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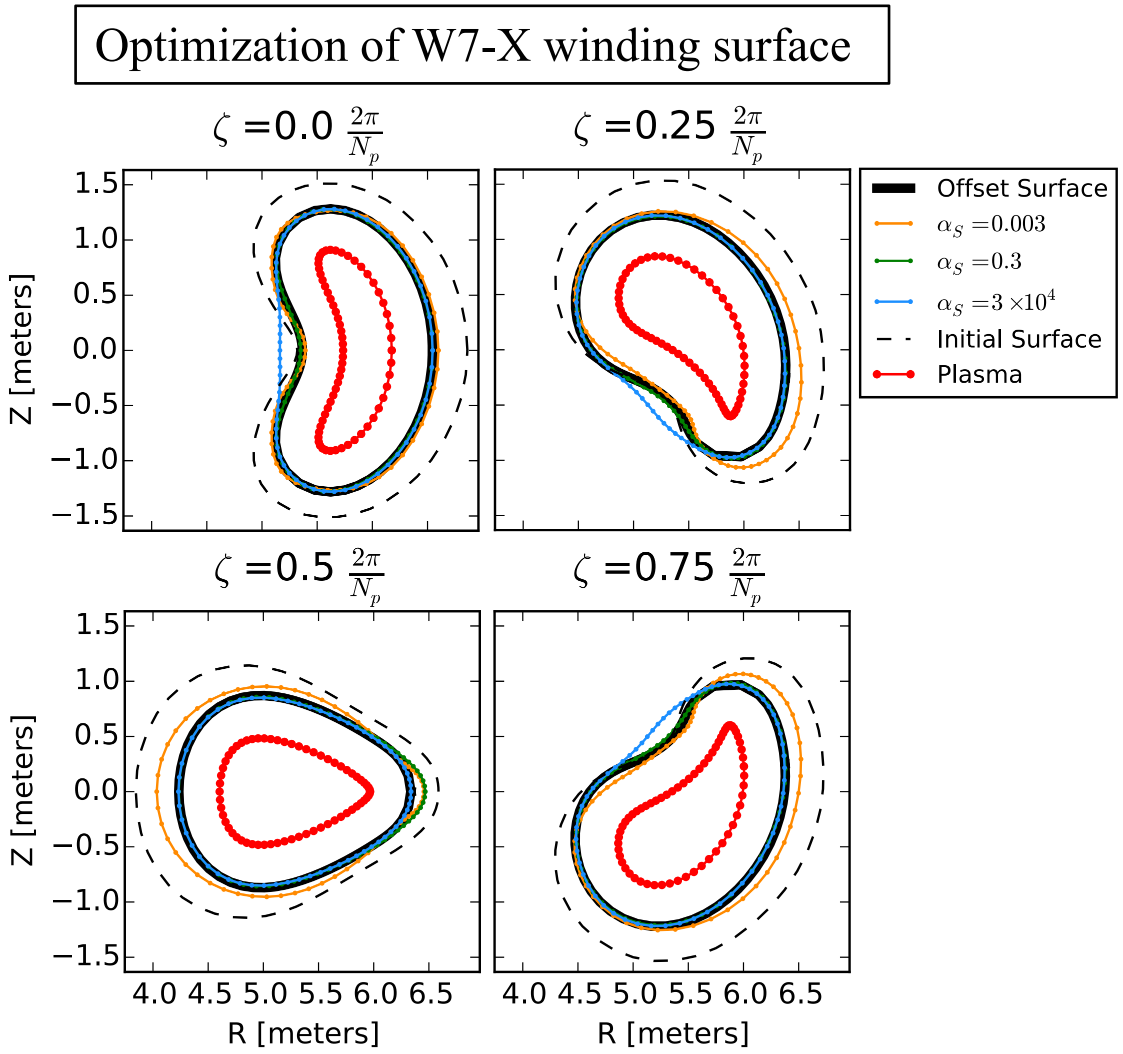
Trends with optimization parameters

$$f = \chi_B^2 + \alpha_S S_p$$



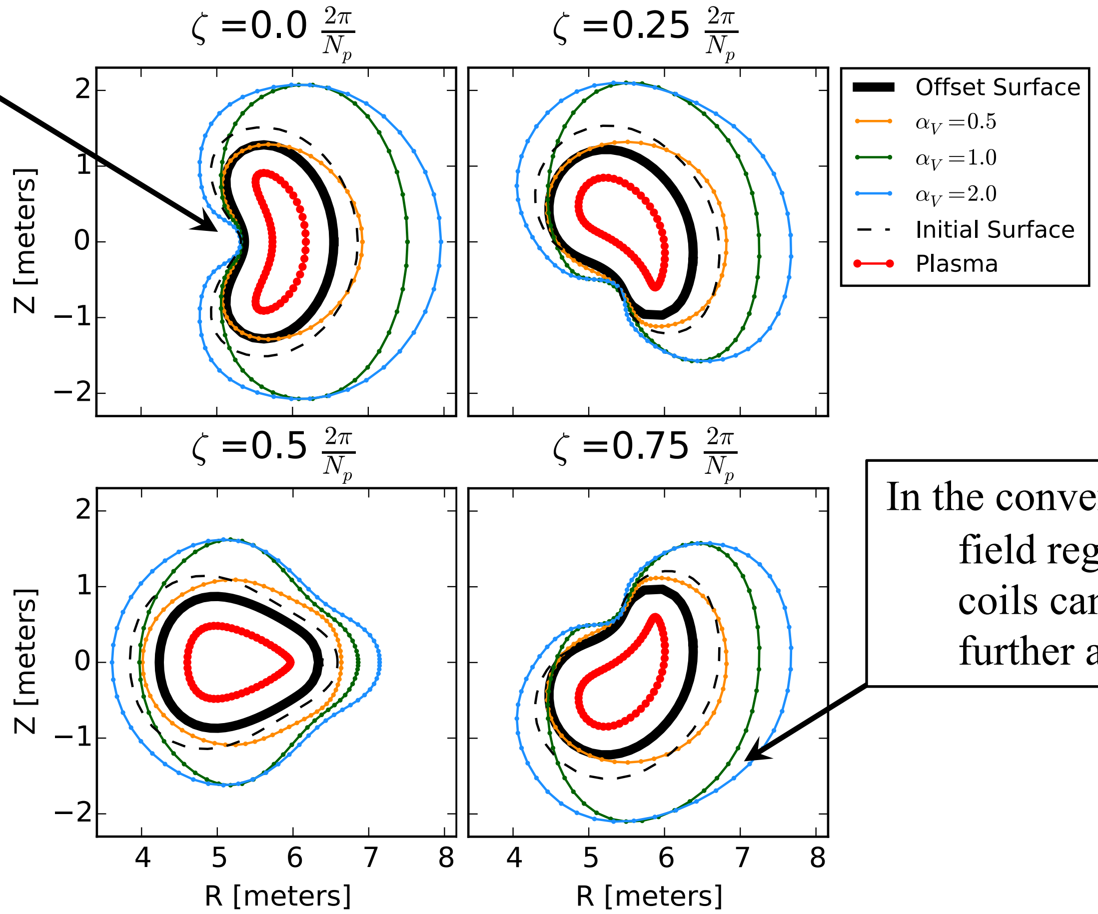
- As α_S increases, winding surfaces approaches cylindrical cross section (minimal Fourier spectrum)
- At moderate α_S, approaches uniform offset from plasma surface (only minimizing χ_B^2)
- Moderate α_S needed to eliminate zero-gradient direction (non-unique parameterization)

$$S_p = \sum_{m,n} m^p \left(\left(r_{mn}^c\right)^2 + \left(z_{mn}^s\right)^2 \right)$$

Trends with optimization parameters

$$f = \chi_B^2 - \alpha_V V_{\text{coil}}^{1/3} + \alpha_S S_p$$

Location of closest approach stays fixed

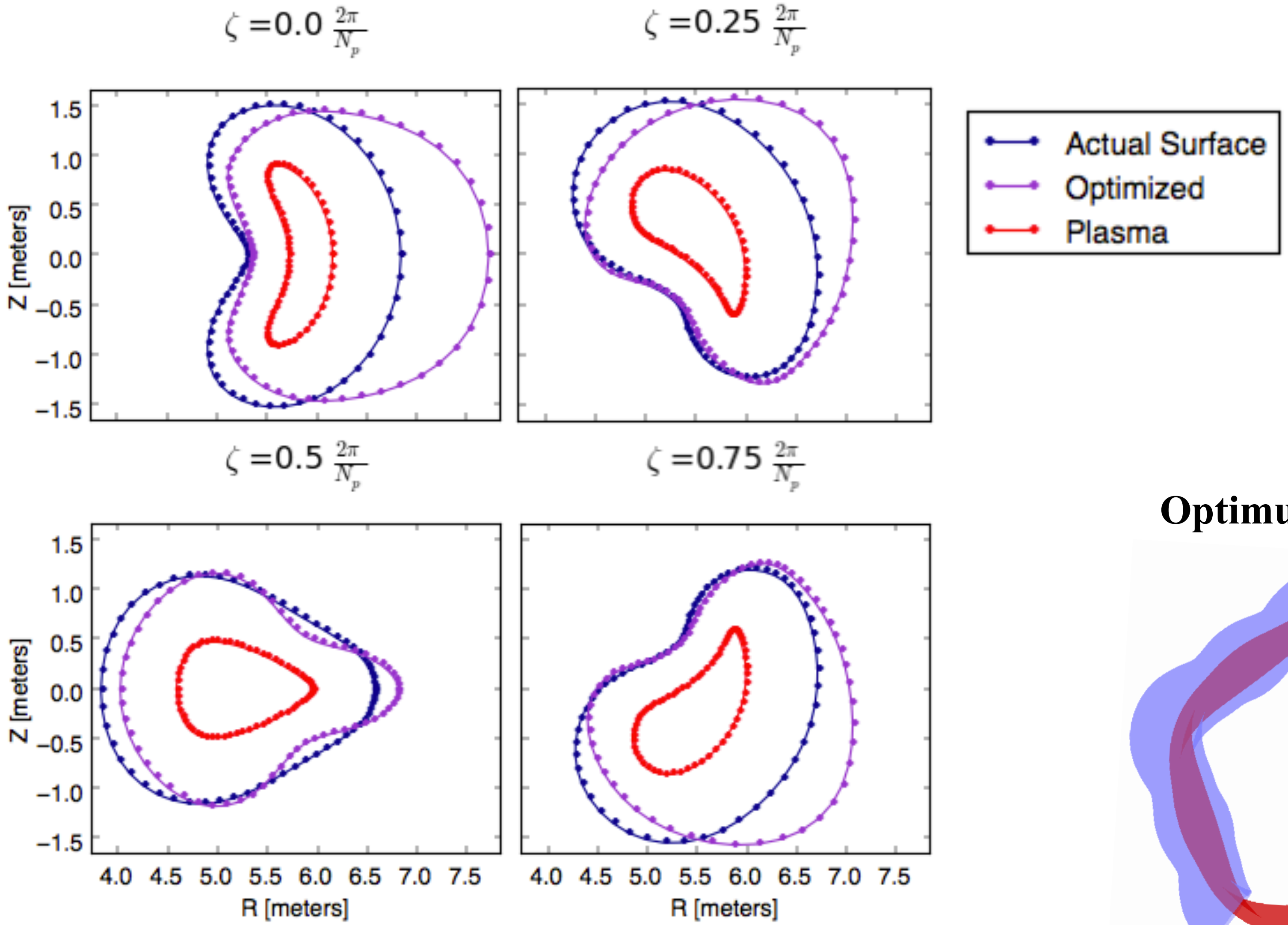


In the convex, low field region, coils can be further away

- $\alpha_S = 0.3$
- As α_V increases, V_{coil} increases
- At small α_V, approaches uniform offset from plasma surface
- Minimum coil-plasma distance remains fixed – needed to produce plasma surface in concave region

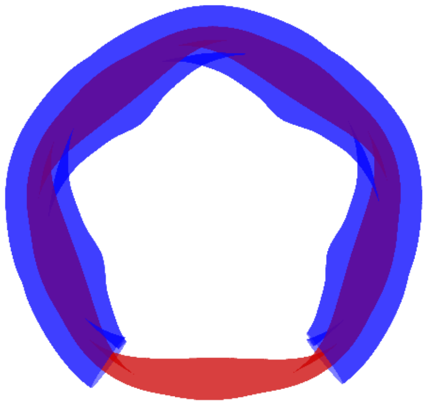
Need to find a balance between the physics (small χ_B^2) and engineering objectives

Optimizing the W7-X winding surface

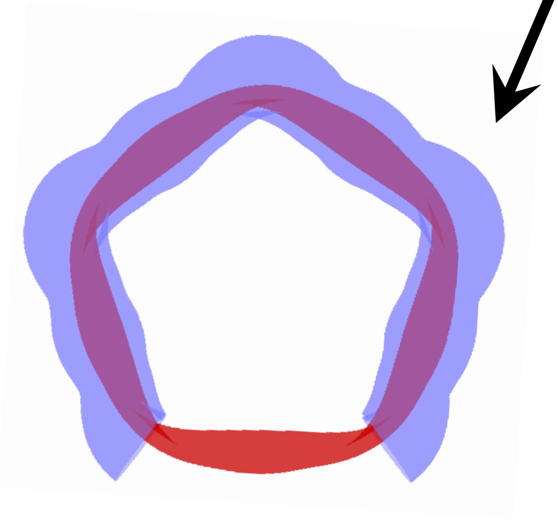


$$\alpha_V = 0.5,\ \alpha_S = 0.24,\ \alpha_K = 1.6 \times 10^{-6}$$

Actual W7-X winding surface (initial surface for optimization)



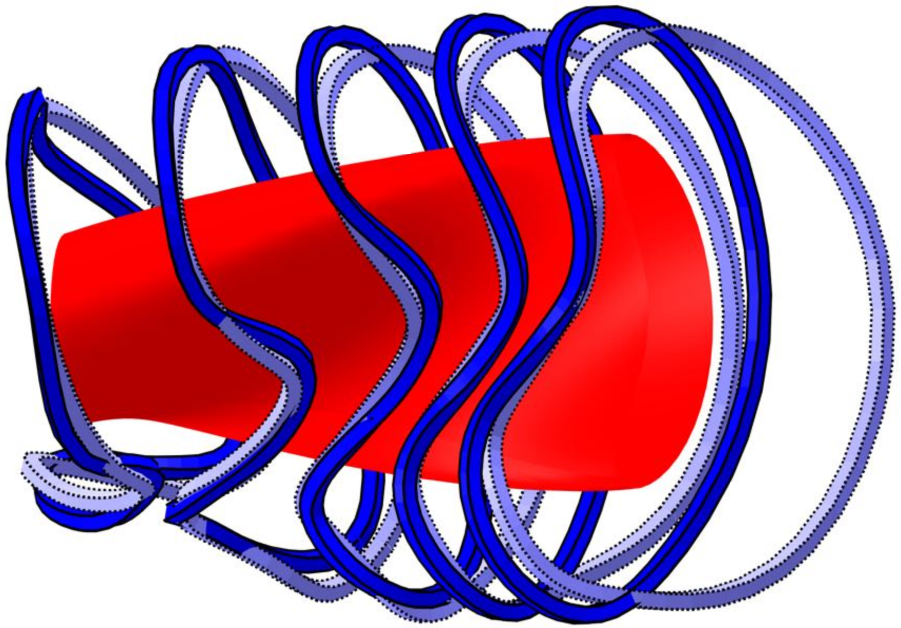
Optimum obtained



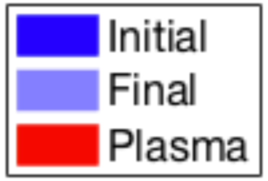
- χ_B^2 decreased 90%
- V_{coil} increased 22%

Optimized W7-X Coils

Side view

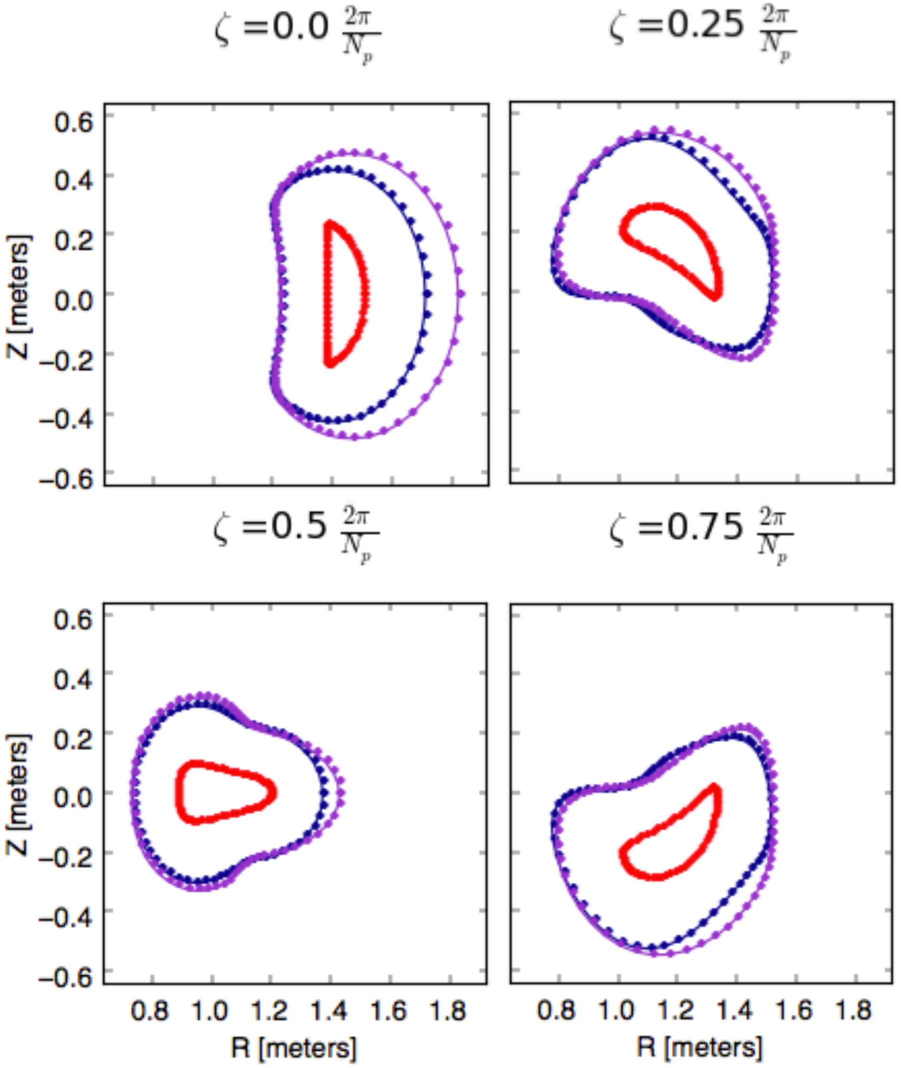


Aerial view



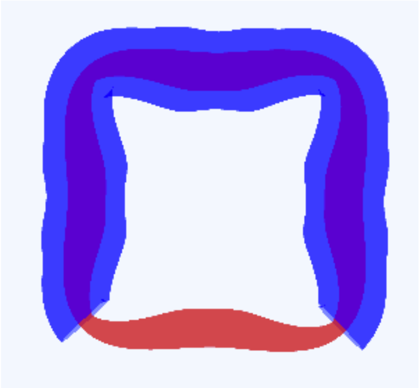
	Initial	**Optimized**
Min. coil-coil distance [m]	0.223	0.271
Max curvature [m^{-1}]	9.01	4.84
Max toroidal extent [rad.]	0.222	0.197

Optimizing the HSX winding surface

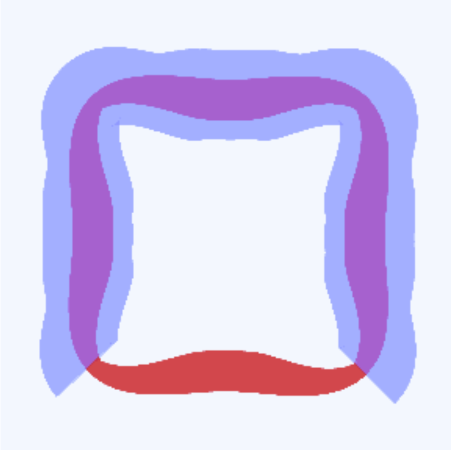


$\alpha_V = 3.13 \times 10^{-4}$, $\alpha_S = 0$, $\alpha_K = 3 \times 10^{-10}$

Actual HSX winding surface (initial surface for optimization)

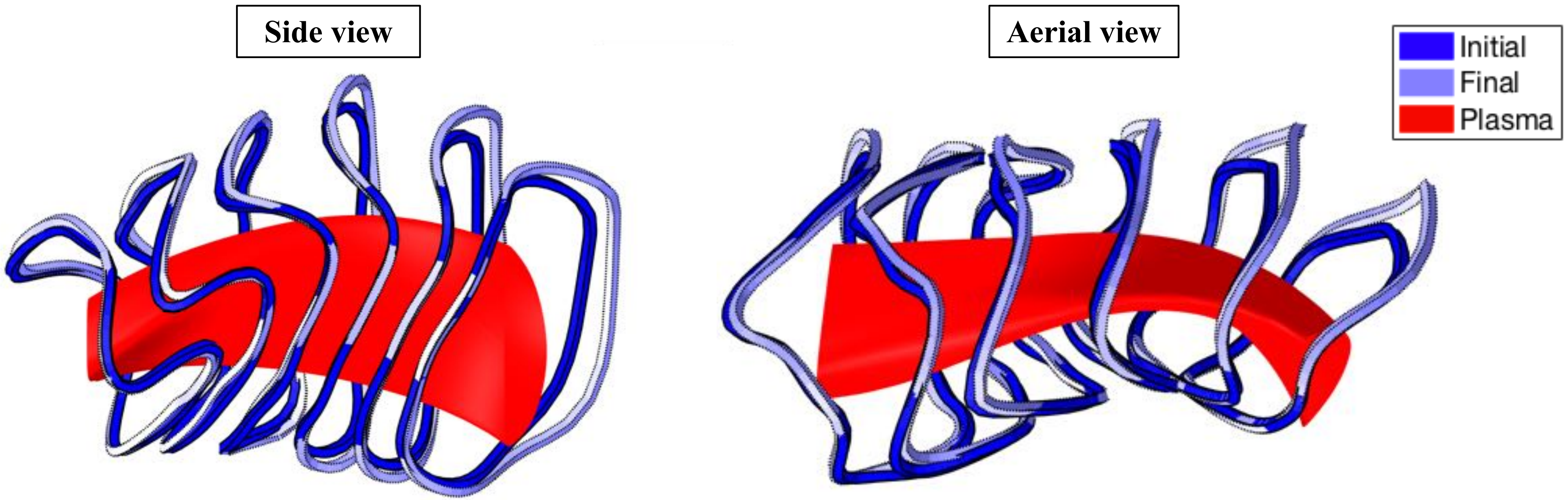


Optimum obtained



- χ_B^2 decreased 33%
- V_{coil} increased 30%

Optimized HSX Coils



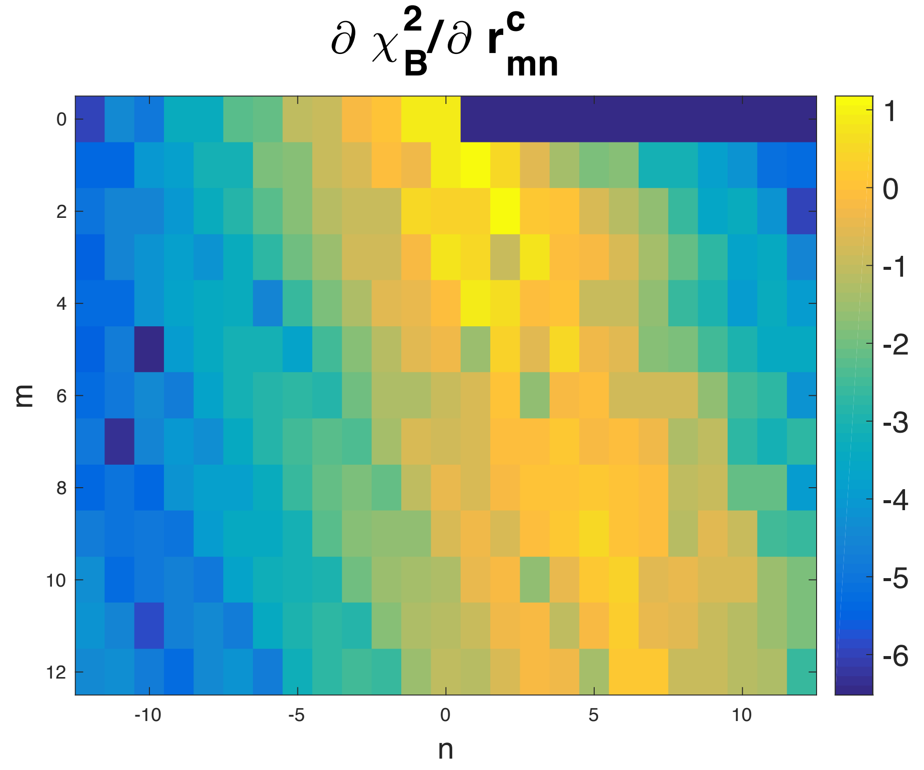
	Initial	Optimized
Min. coil-coil distance [m]	0.0850	0.0853
Max curvature [m^{-1}]	33.4	25.8
Max toroidal extent [rad.]	0.530	0.505

Outline

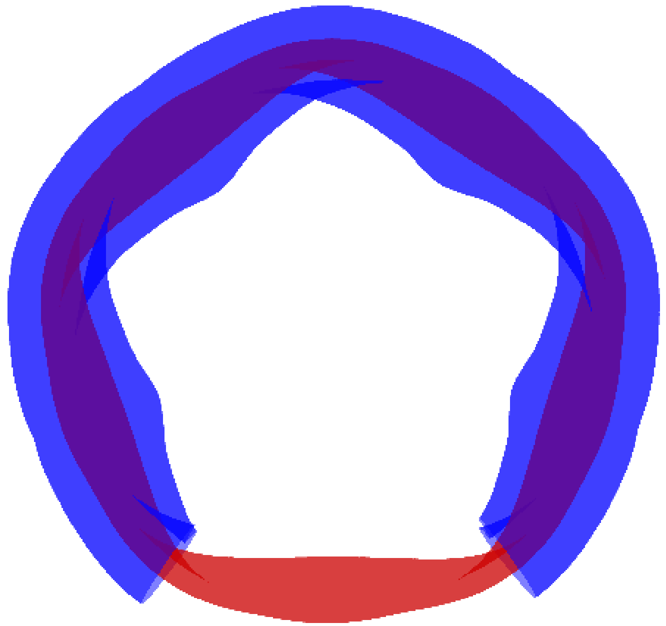
1. Introduction
2. Current potential approach for coil optimization
   a) NESCOIL
   b) REGCOIL
3. Nonlinear optimization of the winding surface
   a) Objective function
   b) Optimization constraints
4. Adjoint method for gradient computation
   a) Examples from CFD and electron gun optimization
   b) Linear adjoint method
5. Applications
   a) Optimization of W7-X and HSX winding surfaces
6. **Local sensitivity analysis**

Computing local sensitivity

"Fourier derivatives" computed using adjoint method



Sensitivity in real space?



Computing local sensitivity with shape gradients

Consider a functional of the shape of some domain, $f(\Gamma)$

Perturbation of domain

$$\Gamma_\epsilon = \{\boldsymbol{r}_0 + \epsilon\delta\boldsymbol{r}(\boldsymbol{r}_0) : \boldsymbol{r}_0 \in \Gamma\}$$

Shape derivative

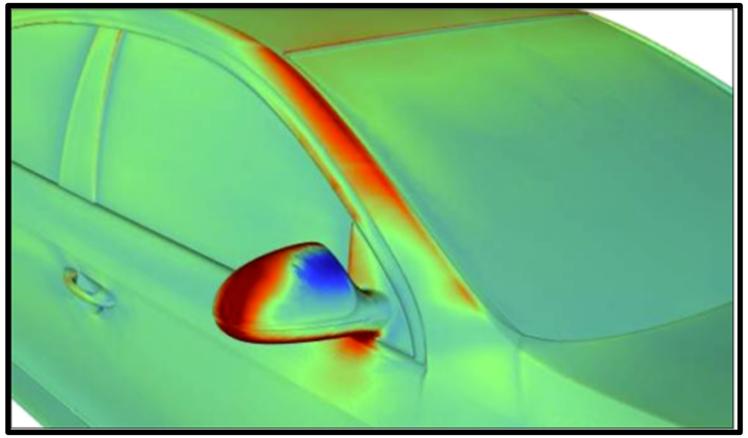
$$\delta f(\Gamma, \delta\boldsymbol{r}) = \lim_{\epsilon \to 0} \frac{f(\Gamma_\epsilon) - f(\Gamma)}{\epsilon}$$

For many functionals, can be written in the 'Hadamard form'

$$\delta f(\Gamma, \delta\boldsymbol{r}) = \int_{\partial\Gamma} d^2A\, S \delta\boldsymbol{r} \cdot \boldsymbol{n}$$

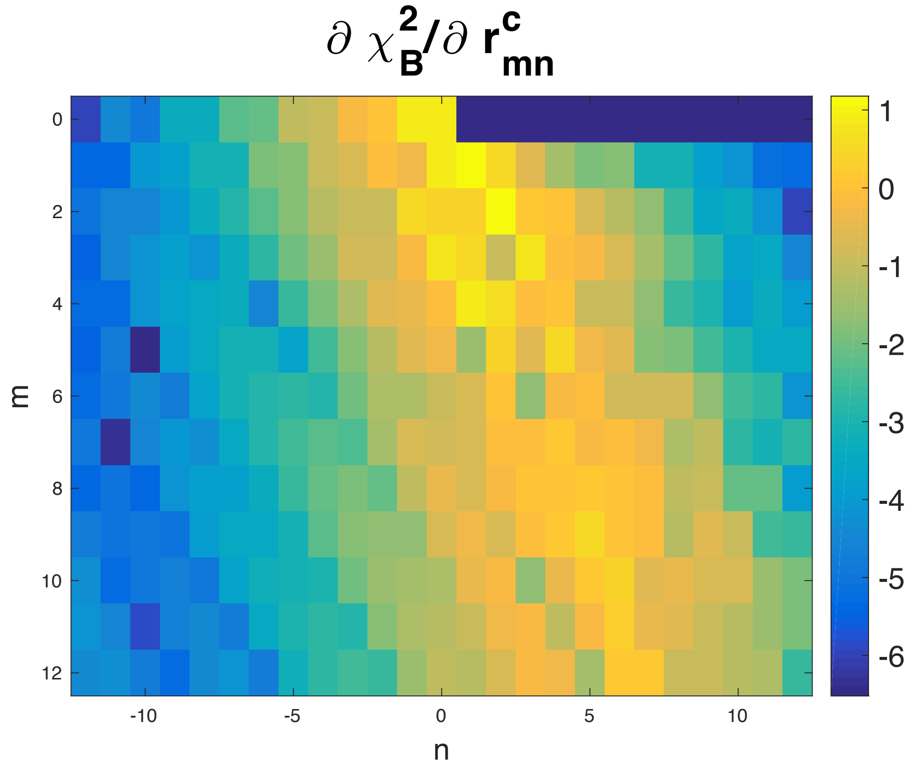
Shape gradient

Shape gradient of drag on a Volkswagon from Navier-Stokes calculations [7]



Computing local sensitivity with shape gradients [13]

"Fourier derivatives" computed using adjoint method



$$\delta\chi^2_B(\Gamma_{\text{coil}}, \delta\boldsymbol{r}) = \int_{\partial\Gamma_{\text{coil}}} d^2A\, S_{\chi^2_B}\, \delta\boldsymbol{r} \cdot \boldsymbol{n}$$

$$S_{\chi^2_B} = \sum_j S_j \cos(m_j\theta - n_j N_p \zeta)$$

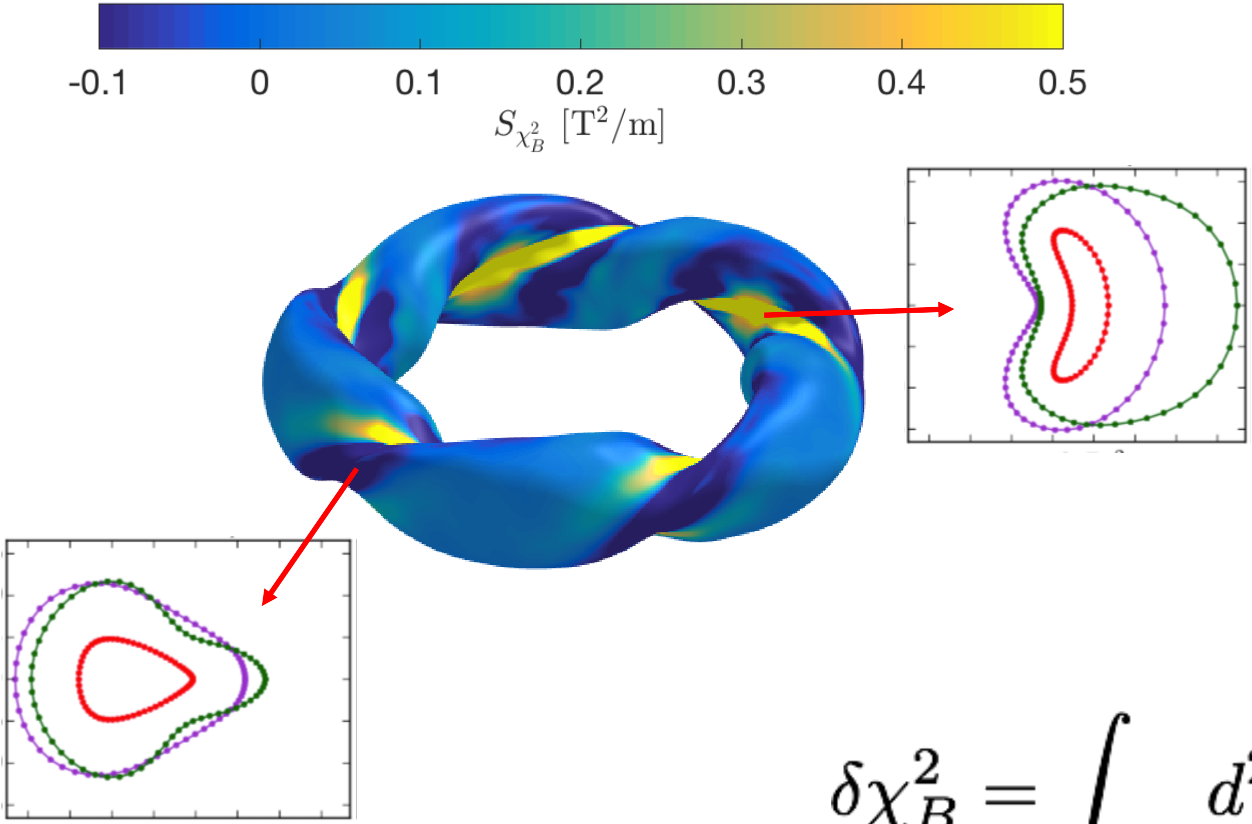
$$\frac{\partial\chi^2_B}{\partial\Omega_i} = \int_{\partial\Gamma_{\text{coil}}} d^2A\, S_{\chi^2_B} \left(\frac{\partial\boldsymbol{r}}{\partial\Omega_i}\right) \cdot \boldsymbol{n}$$

Linear system (generally not square) can be solved with Moore-Penrose pseudoinverse to obtain $S_{\chi^2_B}$

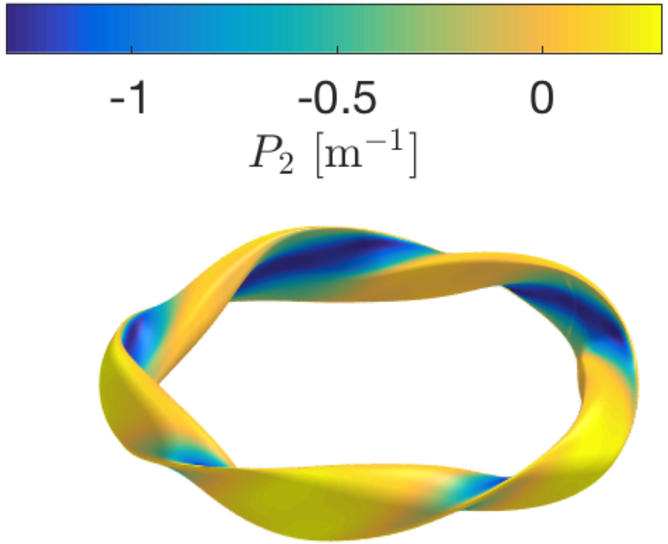
$$\frac{\partial\chi^2_B}{\partial\Omega_i} = \sum_j D_{ij} S_j$$

W7-X winding surface shape gradient

Shape gradient of χ_B^2



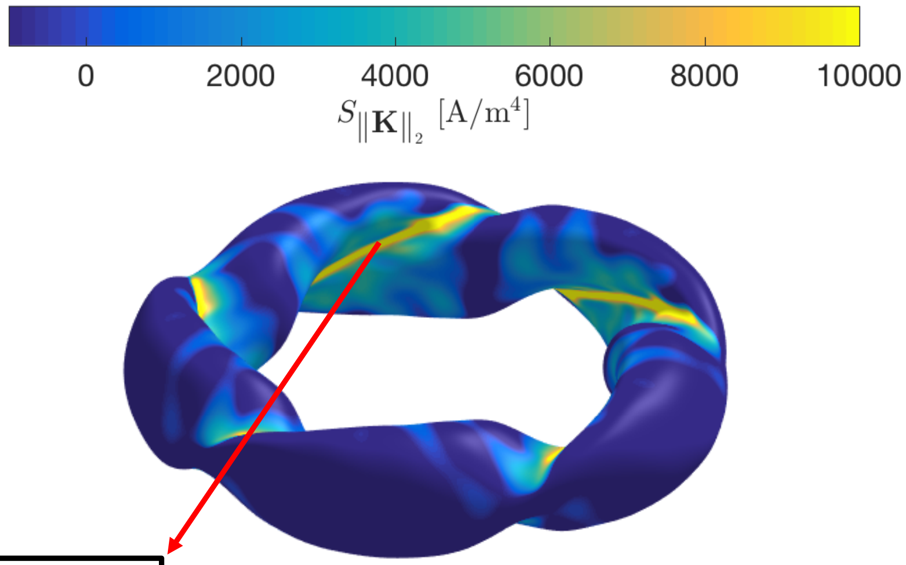
Second principal curvature of plasma surface (negative = concave)

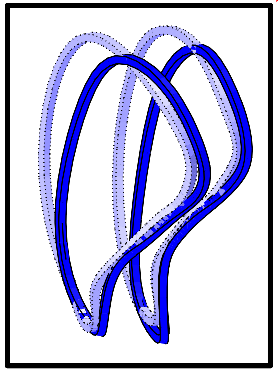


$$\delta \chi_B^2 = \int_{\text{coil}} d^2A \, S_{\chi_B^2} \, \delta \boldsymbol{r} \cdot \boldsymbol{n}$$

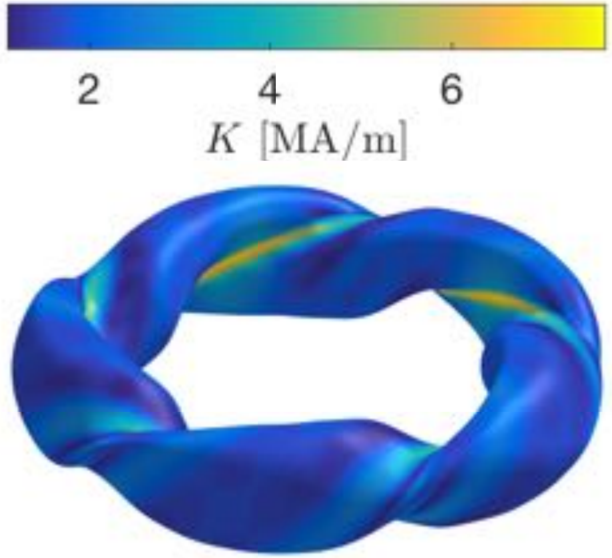
W7-X winding surface shape gradient

Shape gradient of $S_{\|\boldsymbol{K}\|_2}$





Current density



$$\delta \|\boldsymbol{K}\|_2 = \int_{\text{coil}} d^2A \, S_{\|\boldsymbol{K}\|_2} \, \delta \boldsymbol{r} \cdot \boldsymbol{n}$$

Concluding thoughts

- We have demonstrated the first **application of adjoint methods to stellarator coil optimization**
  - Efficient computation of gradients (reduces required function evaluations by a factor of ≈ 50)
- We have obtained winding surfaces for W7-X and HSX which **simultaneously reproduce the desired plasma surfaces with better fidelity, improve engineering properties of coils, and increase the coil-plasma distance**, allowing for more experimental flexibility
- We have developed tools to compute sensitivity to local perturbations of the winding surface

Thank you for your attention!

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